The Energy Eigenvalues of the Two Dimensional Hydrogen Atom in a Magnetic Field

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Abstract

In this paper, the energy eigenvalues of the two dimensional hydrogen atom are presented for the arbitrary Larmor frequencies by using the asymptotic iteration method. We first show the energy eigenvalues for the no magnetic field case analytically, and then we obtain the energy eigenvalues for the strong and weak magnetic field cases within an iterative approach for $n = 2 - 10$ and $m = 0 - 1$ states for several different arbitrary Larmor frequencies. The effect of the magnetic field on the energy eigenvalues is determined precisely. The results are in excellent agreement with the findings of the other methods and our method works for the cases where the others fail.

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I. INTRODUCTION

The study of the two dimensional hydrogen atom in a magnetic field has been a subject of considerable interest over the years. Within the framework of the non-relativistic quantum mechanics, many works have been carried out in order to solve the eigenvalue equation and to find out the correction on the energy eigenvalues in the presence of a constant magnetic field [1, 2, 3, 4, 5]. The solution of this problem is very interesting and popular because of the technological advances in nanofabrication technology which has enabled the creation of low-dimensional structures such as quantum wires, quantum dots and quantum wells in semiconductor physics. Recent developments in nanostructure technology has also permitted one to study the behavior of electrons and impurities in quasi two-dimensional configurations (quantum wells) [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11].

The canonical Hamiltonian for a charge moving in a constant magnetic field can be written as:

$$H = \frac{1}{2\mu}(\mathbf{p} + \frac{e}{c}\mathbf{A})^2 + V(r) \tag{1}$$

where μ is the mass, e is the electric charge, $\mathbf{p}$ is the momentum of the particle, $\mathbf{A}$ is the vector potential, c is the light velocity and V(r) is the cylindrical potential [12]. The hamiltonian for the 2D Hydrogen atom in the magnetic field includes the Coulomb interaction $-Z/r$ between a conduction electron and donor impurity center when a constant $\mathbf{B}$ magnetic field is applied perpendicular to the plane of the motion. If the vector potential in the symmetric gauge is chosen as $\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r}$, the full Hamiltonian for this system can be derived, in the CGS system and in atomic units $\hbar = \mu = e = 1$, as:

$$H = \frac{1}{2}(-i\nabla + \frac{1}{2}\mathbf{B} \times \mathbf{r})^2 - \frac{Z}{r} \tag{2}$$

and the Schrödinger equation becomes

$$H\varphi = \frac{1}{2}(-i\nabla + \frac{1}{2}\mathbf{B} \times \ \mathbf{r})^2\varphi - \frac{Z}{r}\varphi = i\partial_t\varphi = E\varphi \tag{3}$$

Since the problem pertains to two dimensions, it is adequate to study in polar coordinates (r, ϕ) within the plane and to use the following ansatz for the eigenfunction

$$\varphi(r) = \frac{e^{im\phi}}{\sqrt{2\pi}}\frac{R(r)}{\sqrt{r}}, \quad m = 0, \pm 1, \pm 2... \tag{4}$$

Here, the radial wavefunction $R(r)$ must satisfy the following radial Schrödinger equation:

$$\frac{d^2R(r)}{dr^2} + 2\left[(E - m\omega_L) - \frac{(m^2 - \frac{1}{4})}{2r^2} - \frac{1}{2}\omega_L^2 r^2 + \frac{Z}{r}\right] R(r) = 0 \tag{5}$$

where $\omega_L = B/2c$ is the Larmor frequency, E is the energy eigenvalue and m is the eigenvalue of the angular momentum.

As it is seen from equation (5), we need an effective potential of $\alpha r^{-2} + \beta r^{-1} + \gamma r^2$ type, which is a hybrid of Coulomb plus harmonic oscillator potential, in order to describe the two dimensional hydrogen atom in a magnetic field. This potential can not be solved analytically except for particular cases and there are no general closed form solutions to equation (5) in terms of the special functions [13]. There are analytic expressions for the eigenvalues for particular values of w_L and m [14, 15].

Therefore, in this paper, in order to find the energy eigenvalues for the two dimensional hydrogen atom in a constant magnetic field with the arbitrary Larmor frequencies w_L [16, 17, 18, 19], we use a more practical and systematic method, called the Asymptotic Iteration Method (AIM) for different n and m quantum numbers. This is precisely the aim of this paper.

In the next section, we briefly outline AIM with all necessary formulae to perform our calculations. In section III, we first apply AIM to solve the Schrödinger equation for the case $\omega_L = 0$: no magnetic field and to obtain an analytical expression for any n and m states. Then, we show how to solve the resulting Schrödinger equation for the case $w_L \neq 0$: strong and weak magnetic fields where there are no analytical solutions. Here, for any n and m quantum numbers, we show the effect of the magnetic field on the energy eigenvalues and compare our results with the findings of other methods [15]. Finally, section IV is devoted to our summary and conclusion.

II. BASIC EQUATIONS OF THE ASYMPTOTIC ITERATION METHOD (AIM)

AIM is proposed to solve the second-order differential equations of the form [20, 21, 22].

$$y'' = \lambda_0(x)y' + s_0(x)y \tag{6}$$

where $\lambda_0(x) \neq 0$ and the functions, $s_0(x)$ and $\lambda_0(x)$, are sufficiently differentiable. The differential equation (6) has a general solution [20]

$$y(x) = exp\left(-\int^x \alpha(x^{'})dx^{'}\right)\left[C_2 + C_1\int^x exp\left(\int^{x^{'}}(\lambda_0(x^{''}) + 2\alpha(x^{''}))dx^{''}\right)dx^{'}\right] \tag{7}$$

if $k > 0$, for sufficiently large k, we obtain the $\alpha(x)$ values from

$$\frac{s_k(x)}{\lambda_k(x)} = \frac{s_{k-1}(x)}{\lambda_{k-1}(x)} = \alpha(x), \quad k = 1, 2, 3, \ldots \tag{8}$$

where

$$\begin{aligned} \lambda_k(x) &= \lambda'_{k-1}(x) + s_{k-1}(x) + \lambda_0(x)\lambda_{k-1}(x) \\ s_k(x) &= s'_{k-1}(x) + s_0(x)\lambda_{k-1}(x), \qquad k = 1, 2, 3, \ldots \end{aligned} \tag{9}$$

The energy eigenvalues are obtained from the quantization condition. The quantization condition of the method together with equation (9) can also be written as follows

$$\delta_k(x) = \lambda_k(x)s_{k-1}(x) - \lambda_{k-1}(x)s_k(x) = 0, \qquad k = 1, 2, 3, \ldots \tag{10}$$

For a given potential, the radial Schrödinger equation is converted to the form of equation (6). Then, $s_0(x)$ and $\lambda_0(x)$ are determined and $s_k(x)$ and $\lambda_k(x)$ parameters are calculated by using equation (9). The energy eigenvalues are determined by the quantization condition given by equation (10).

III. AIM SOLUTION FOR THE TWO DIMENSIONAL HYDROGEN ATOM

Applying the scale transformation $r = r_0\rho \quad (r_0 = \frac{1}{2Z})$ to equation (5) and by using the following *ansatz*:

$$\varepsilon = \frac{(E - m\omega_L)}{2Z^2}, \quad \beta^2 = \frac{\omega_L^2}{16Z^4}, \qquad l'(l'+1) = m^2 - \frac{1}{4} \tag{11}$$

we can easily find

$$\frac{d^2R(\rho)}{d\rho^2} + \left[\varepsilon + \frac{1}{\rho} - \beta^2\rho^2 - \frac{l'(l'+1)}{\rho^2}\right]R(\rho) = 0 \tag{12}$$

In what follows, we show how to obtain the energy eigenvalues from this equation for two different cases, depending on the values of ω_L and show the effect of the ω_L on the eigenvalues.

A. Case $\omega_L = 0$: no magnetic field

When $\omega_L = 0$, equation (12) becomes

$$\frac{d^2R(\rho)}{d\rho^2} + \left[-\varepsilon'^2 + \frac{1}{\rho} - \frac{l'(l'+1)}{\rho^2}\right] R(\rho) = 0 \tag{13}$$

where $-\varepsilon'^2 = \frac{(E-m\omega_L)}{2Z^2}$. In order to solve this equation with AIM, we should transform this equation to the form of equation (6). Therefore, the reasonable physical wave function we propose is as follows

$$R(\rho) = \rho^{l'+1} e^{-\varepsilon'\rho} f(\rho) \tag{14}$$

equating it into equation (13) leads to

$$\frac{d^2f(\rho)}{d\rho^2} = \left(\frac{2\varepsilon'\rho - 2l' - 2}{\rho}\right)\frac{df(\rho)}{d\rho} + \left(\frac{2\varepsilon' l' + 2\varepsilon' - 1}{\rho}\right) f(\rho) \tag{15}$$

where $\lambda_0 = 2(\frac{\varepsilon'\rho - l' - 1}{\rho})$ and $s_0 = \frac{2\varepsilon' l' + 2\varepsilon' - 1}{\rho}$. By means of equation(9), we may calculate $\lambda_k(\rho)$ and $s_k(\rho)$. This gives

$$\begin{aligned}
\lambda_0 &= 2\left(\frac{\varepsilon'\rho - l' - 1}{\rho}\right) \\
s_0 &= \frac{2\varepsilon' l' + 2\varepsilon' - 1}{\rho} \\
\lambda_1 &= \frac{10l' + 6 - 6\rho\varepsilon' l' - 6\varepsilon'\rho - \rho + 4\varepsilon'^2\rho^2 + 4l'^2}{\rho^2} \\
s_1 &= \frac{-10\varepsilon' l' - 6\varepsilon' + 3 + 4\varepsilon'^2 l'\rho - 4\varepsilon' l'^2 + 4\varepsilon'^2\rho - 2\varepsilon'\rho + 2l'}{\rho^2} \\
&...etc
\end{aligned} \tag{16}$$

Combining these results with the quantization condition given by equation (10) yields

$$\begin{aligned}
\frac{s_0}{\lambda_0} &= \frac{s_1}{\lambda_1} \quad \Rightarrow \quad (\varepsilon')_0 = \frac{1}{2(l'+1)} \\
\frac{s_1}{\lambda_1} &= \frac{s_2}{\lambda_2} \quad \Rightarrow \quad (\varepsilon')_1 = \frac{1}{2(l'+2)} \\
\frac{s_2}{\lambda_2} &= \frac{s_3}{\lambda_3} \quad \Rightarrow \quad (\varepsilon')_2 = \frac{1}{2(l'+3)} \\
&\ldots etc
\end{aligned} \tag{17}$$

If the above expressions are generalized, ε' turns out as

$$(\varepsilon')_n = \frac{1}{2(l'+n+1)} \qquad\qquad n = 0, 1, 2, 3... \tag{18}$$

If one inserts values of ε' and l' into equation (18), the eigenvalues of the $2D$ hydrogen atom in the case $w_L = 0$ becomes

$$E_n = -\frac{1}{2(|m| + n + \frac{1}{2})^2} \tag{19}$$

This analytical formula is in agreement with the previous works [12]. We discuss the results of the $w_L = 0$ case together with the findings of the case $w_L \neq 0$ in the next subsection.

B. Case $w_L \neq 0$: strong and weak magnetic fields

Before applying AIM to this problem, we have to obtain asymptotic wavefunction and then transform equation (12) to an amenable form for AIM. We transform equation (12) to another Schrödinger form by changing the variable as $\rho = u^2$ and then by inserting $R(u) = u^{1/2}\chi(u)$ into the transformed equation. Thus, we get another Schrödinger form which is more suitable for an AIM solution:

$$\frac{d^2\chi(u)}{du^2} + \left[4\varepsilon u^2 + 4 - 4\beta^2 u^6 - \frac{\Lambda(\Lambda+1)}{u^2}\right]\chi(u) = 0 \tag{20}$$

where $\Lambda = 2l' + \frac{1}{2}$. It is clear that when u goes to zero, $\chi(u)$ behaves like $u^{\Lambda+1}$ and $\exp\left(-\frac{\alpha}{4}u^4\right)$ at infinity, therefore, the wavefunction for this problem can be written as follows:

$$\chi(u) = u^{\Lambda+1}\exp\left(-\frac{\alpha}{4}u^4\right) f(u) \tag{21}$$

If this wave function is inserted into equation (20), we have the second-order homogeneous linear differential equation in the following form

$$f'' = 2\left(\alpha u^3 - \frac{\Lambda+1}{u}\right) f' + \left(\left[(2\Lambda+5)\,\alpha - 4\varepsilon\right] u^2 - 4\right) f \tag{22}$$

Where $\alpha = 2\beta$. By comparing this equation with equation (6), $\lambda_0(u)$ and $s_0(u)$ values can be written as below

$$\lambda_0 = 2\left(\alpha u^3 - \frac{\Lambda+1}{u}\right), \qquad s_0 = \left[(2\Lambda+5)\,\alpha - 4\varepsilon\right] u^2 - 4 \tag{23}$$

In AIM, we calculate the energy eigenvalues from the quantization condition given by equation (10). It is important to point out that the problem is called "exactly solvable" if this equation is solvable at every u point. In our case, since the problem is not exactly solvable, we have to choose a suitable u_0 point and to solve the equation $\delta_k(u_0, \varepsilon) = 0$ to

find ε values. In this work, we obtain the u_0 from the maximum point of the asymptotic wavefunction which is the same as the root of $\lambda_0(u) = 0$, thus $u_0 = \left(\frac{\Lambda+1}{\alpha}\right)^{1/4}$. The results obtained by using AIM are shown in Tables I and II in comparison with the results of Ref. [15] for $Z = 1$, $n = 2-10$, $m = 0$ and $m = 1$ with different Larmor frequencies ω_L. Ref. [15] was able to solve this equation analytically for particular values of ω_L, n and m quantum numbers. However, he could not obtain the ground state energy eigenvalue and the energy eigenvalues also diverged for ω_L=0: No solution could be obtained. In Table III, we have shown the eigenvalues for several Larmor frequencies for the ground state and second excited states, which could not be obtained by Ref. [15]. In order to show that our method can obtain energy eigenvalues for arbitrary Larmor frequencies, we have calculated the energy eigenvalues for a few arbitrary Larmor frequencies with $m = 0$, $m = 1$ and $n = 1 - 3$ values in Tables IV and V. The first lines of Tables IV and V show the results for the case $w_L = 0$ with different quantum numbers n and m. We present only $m = 0$, $m = 1$ and $n = 1$ to 3 for illustration, but any value of n and m can be obtained.

IV. CONCLUSION

In this paper, we have shown an alternative method to obtain the energy eigenvalues for the two dimensional hydrogen atom without the magnetic field and in a constant magnetic field for arbitrary Larmor frequencies for various n and m quantum numbers within the framework of the asymptotic iteration method. We have first applied AIM to solve the radial Schrödinger equation for the case $\omega_L = 0$: no magnetic field and have obtained an analytical expression for the energy eigenvalues for any n and m states. Then, we have shown how to solve the resulting radial Schrödinger equation for the case $w_L \neq 0$: strong and weak magnetic fields. This equation cannot be solved analytically, therefore, we have shown how to obtain the energy eigenvalues by an iterative approach within the framework of AIM. By comparing these two cases ($w_L = 0$ and $w_L \neq 0$), we have shown the effect of the magnetic field on the energy eigenvalues in the tables and have compared our results with the findings of other methods.

Besides showing the applicability of a new method to solve the radial Schrödinger equation in the magnetic field for any n and m quantum numbers, one of the novelties of this paper is that we have shown that it is possible to obtain the ground state energy eigenvalues where

others works such as [15] have failed to obtain. We have also shown that it is possible to solve the $w_L = 0$ and $w_L \neq 0$ case simultaneously where, in general, the $w_L = 0$ case makes the energy eigenvalues diverge and non-physical results are obtained (see Ref. [15] for details.)

It is clearly shown in this paper that the method presented in this study is a systematic one and it is very efficient and practical to obtain the eigenvalues for the Schrödinger type equations in a magnetic field and without the magnetic field. It is worth extending this method to the solution of other problems.

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$m = 0$

n	ω_L^{-1}	E[15]	E_{AIM}
2	0.50000	4.0000000	4.0000000
3	3.00000	1.0000000	1.0000000
4	9.27200	0.4314060	0.4314064
	0.727998	5.4945200	5.4945207
5	21.1168	0.2367780	0.2367785
	3.88316	1.2876100	1.2876109
6	40.3133	0.1488340	0.1488343
	11.2570	0.5330000	0.5330020
	0.929632	6.4541700	6.4541668
7	68.6380	0.1019840	0.1019840
	24.6751	0.2836870	0.2836867
	4.68692	1.4935200	1.4935182
8	107.868	0.0741648	0.0741647
	45.9214	0.1742110	0.1742107
	13.0953	0.6109080	0.6109059
	1.11539	7.1723900	7.1723786
9	159.781	0.0563272	0.0563271
	76.7724	0.1172300	0.1172296
	28.0095	0.3213200	0.3213195
	5.43732	1.6552300	1.6552272
10	226.154	0.0442176	0.0442177
	119.005	0.0840301	0.0840301
	51.2233	0.1952240	0.1952236
	14.8274	0.6744290	0.6744268
	1.29016	7.7509600	7.7509774

TABLE I: The energy eigenvalues obtained by using AIM for all allowed Larmor frequencies ω_L used by Ref. [15] for $Z = 1$, $n = 2 - 10$ and $m = 0$.

$m = 1$

n	ω_L^{-1}	E[15]	E_{AIM}
2	1.50000	2.6666700	2.6666667
3	7.00000	0.7142860	0.7142857
4	18.1394	0.3307720	0.3307717
	1.86059	3.2247800	3.2247835
5	36.6810	0.1909910	0.1907883
	8.34903	0.8384210	0.8384207
6	64.2985	0.1244200	0.1244197
	21.0161	0.3806600	0.3806606
	2.18539	3.6606800	3.6606737
7	102.855	0.0875018	0.0875018
	41.5559	0.2165760	0.2165757
	9.58910	0.9385660	0.9385656
8	154.096	0.0648944	0.0648947
	71.7176	0.1394360	0.1394358
	23.6998	0.4219450	0.4219444
	2.48615	4.0222800	4.0222838
9	219.800	0.0500456	0.0500455
	113.269	0.0971138	0.0971140
	46.1803	0.2381970	0.2381968
	10.7509	1.0231700	1.0231700
10	301.742	0.0397691	0.0397691
	167.984	0.0714353	0.0714354
	78.7673	0.1523470	0.1523475
	26.2373	0.4573650	0.4573641
	2.76930	4.3332300	4.3332248

TABLE II: The same as table I, but for $m = 1$.

ω_L^{-1}	m	n	E[15]	E_{AIM}
0.50000	0	1	-	-1.459586
		2	4.00000	4.000000
		3	-	8.344348
3.00000	0	1	-	-1.979604
		2	-	0.180700
		3	1.00000	1.000000
1.50000	1	1	-	1.200118
		2	2.66667	2.666666
		3	-	4.070242
7.00000	1	1	-	0.002497
		2	-	0.387686
		3	0.714286	0.714285

TABLE III: Several Larmor frequencies ω_L and corresponding eigenvalues E in $Z = 1$, $n = 2 - 10$ and $m = 0 - 1$ and where $n = 1$ is the ground state

.

$m = 0$

w_L	$n = 1$	$n = 2$	$n = 3$
0	-2.000000	-0.222222	-0.08000
0.050	-1.999530	-0.205286	0.001634
0.125	-1.997078	-0.135464	0.227218
0.214	-1.991490	-0.015458	0.541870
0.333	-1.979644	0.180112	0.998682
0.500	-1.955159	0.494679	1.676971
0.750	-1.903352	1.017056	2.737039
1.166	-1.784478	1.962502	4.564444
2.000	-1.459586	4.000000	8.344352
4.500	-0.121100	10.538252	20.029864

TABLE IV: Corresponding eigenvalues for $w_L = 0$: no magnetic field and for the arbitrary Larmor frequencies for the values of $m = 0$ and $n = 1 - 3$, where n=1 is ground state, $n = 2$ is the first excited state, $n = 3$ is the second excited state.

$m = 1$

w_L	$n = 1$	$n = 2$	$n = 3$
0	-0.222222	-0.080000	-0.040816
0.050	-0.159232	0.043578	0.174858
0.125	-0.031456	0.317382	0.60668
0.214	0.146176	0.677668	1.152122
0.333	0.406240	1.183896	1.903978
0.500	0.795208	1.918102	2.980934
0.750	1.406898	3.044950	4.61856
1.166	2.467582	4.959271	7.379467
2.000	4.675218	8.870088	12.981222
4.500	11.550624	20.821926	29.981774

TABLE V: The same as table IV, but for $m = 1$.